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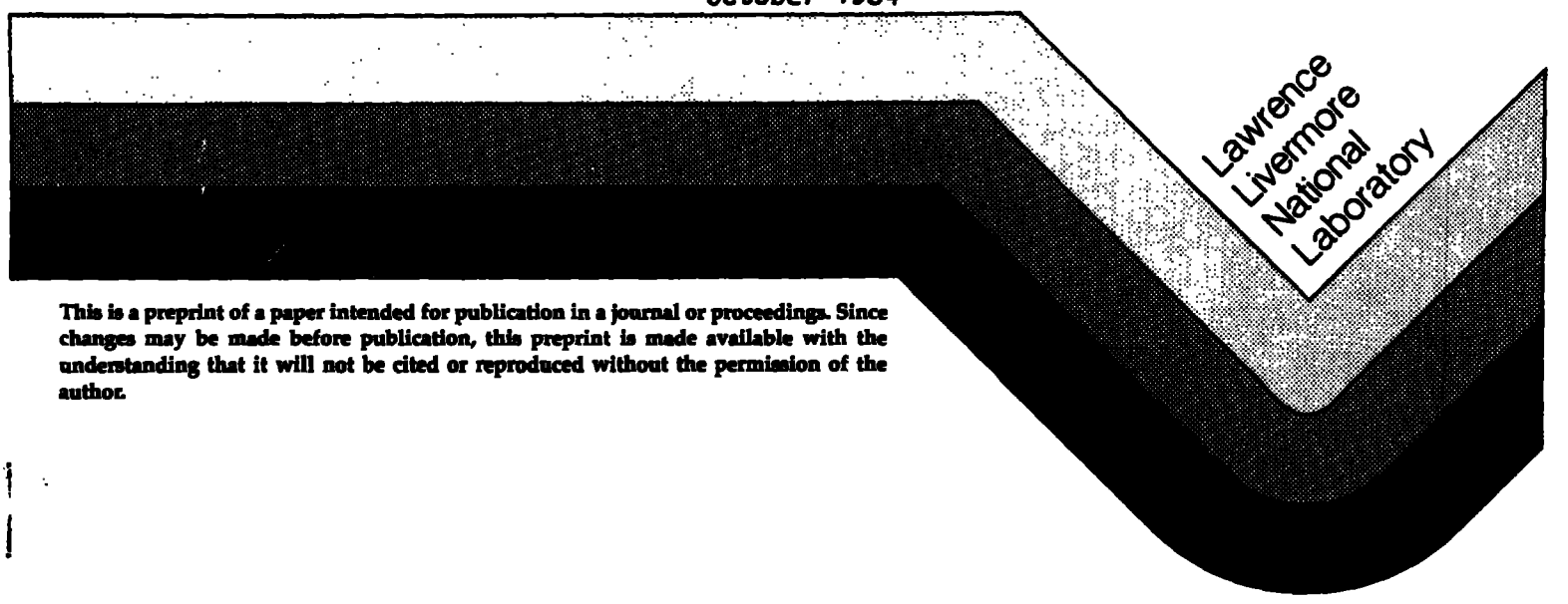

# ELECTRON CHANNELING RADIATION FROM DIAMONDS WITH AND WITHOUT PLATELETS

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## ABSTRACT

Channeling-radiation spectra produced by planar-channeled, 30.5-MeV electrons in Type-Ia and Type-IIa natural diamonds have been measured and are compared with previous results for 54.5-MeV electrons. Because of the presence of platelets precipitated along the (100) planes in the Type-Ia diamond, the energies of the (100) spectral peaks are shifted downward relative to those for the Type-IIa diamond. We have developed a model to explain this effect.

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# I. INTRODUCTION

In a previous paper[1] we presented experimental data for the channeling radiation produced by 54.5-MeV electrons and positrons in Type-Ia and Type-IIa natural diamonds. Type-Ia diamonds contain platelets precipitated along the (100) planes; type-IIa diamonds do not. For both electrons and positrons, the spectral features (peak energies, linewidths, and intensities) of the two types were different. Perhaps the most interesting feature is the downshift in energy of the spectral peaks for electrons incident along the (100) plane in the Type-Ia diamond relative to those for the Type-IIa diamond. In this paper we present a model to explain this observation, along with additional data obtained for 30.5-MeV channeled electrons.[2]

More extensive measurements on the Type-IIa diamond have been presented and discussed in detail in Ref. 3. The first channeling-radiation data reported for diamond in this energy range were obtained at Saclay using a nearly defect-free portion of a synthetic diamond.[4]

Ninety-eight percent of all natural diamonds are of Type Ia and only about 1% are of Type IIa. Type-Ia diamonds contain platelets, which apparently are interplanar aggregates of atoms, at least partly nitrogen, precipitated during the cooling phase of their growth along (100) planes in single or double layers. Evans[5] summarized the properties of platelets as they were known in 1976. Models of platelets as (a) double layers of predominantly nitrogen atoms or (b) single layers of predominantly carbon (but possibly nitrogen) atoms have been proposed by Lang[6] and Humble,[7] respectively. Barry et al.[8] have proposed a new "zig-zag" model, which is similar to the Lang model in its use of double layers of nitrogen atoms but is different in the details of their structure and spacing. A recent

measurement[9] using high-resolution electron energy-loss spectroscopy has shown conclusively that nitrogen is a major constituent of platelets. Of greater significance to the present work, however, is the displacement of the (100) planes which results from the presence of a platelet. The Lang model, pictured in Fig. 1(a), gives a total displacement of a/3, where a = 3.567 Å is the lattice constant for diamond. The Humble model, pictured in Fig. 1(b), gives a total displacement of 0.4a. More recent analyses have yielded values of 0.35a (Ref. 10) and (0.33 ± 0.05)a (Ref. 11). Further details of the related structural properties of diamonds can be found in Refs. 12 and 13.

Along the (111) planes, the platelets disrupt the crystal structure in much the same way as do stacking faults, displacing the planes by a distance equal to $1/\sqrt{3}$ of the displacement of the (100) planes. A similar situation pertains to the (110) planes, except that for this case the displacement is equal to $1/\sqrt{2}$ of the displacement of the (100) planes. Along the (100) planes, on the other hand, it can be seen from Fig. 1 that the platelets cause a distortion (rather than a disruption) of the crystal structure.

## II. EXPERIMENTAL RESULTS

The experiment was performed with a 30.5-MeV electron beam from the Lawrence Livermore National Laboratory Electron-Positron Linear Accelerator. A comprehensive summary of the details of the experimental apparatus and techniques, together with the details of the calculational methods we use to compare theoretical and experimental results, is given in Ref. 3.

The 12-μm-thick Type-Ia diamond was cut normal to its <110> axis and the 23-μm-thick Type-IIa diamond was cut normal to its <100> axis. Transmission-electron-microscopy photographs of the Type-Ia diamond showed platelet diameters that varied from 40 Å to over 200 Å, with an average separation of ∿500 Å. From an infrared-absorption measurement, we estimate (see Ref. 13) that the mean separation between platelet encounters for a planar-channeled electron is ∿4500 Å.

The radiation spectra from 30.5-MeV electrons channeled along the three major planes of diamond are shown in Fig. 2. These results were obtained by subtracting the bremsstrahlung spectra produced when the orientation of the crystal was in a random direction relative to the electron-beam direction from those when it was aligned along a major craystal plane. In each part of the figure, two spectra are superposed, corresponding to the two diamonds used. These two spectra were normalized to each other by matching the photon yields in the 500-to-700-keV photon-energy region.

The parameters of the spectral peaks are listed in Table I. For the (111) plane [Fig. 2(a)], the effect of the platelets is a modest decrease in intensity, whereas for the (110) plane [Fig. 2(b)], the reduction in intensity caused by the platelets is so severe that no individual spectral lines can be discerned. Both of these effects can be explained in terms of the heuristic

model of Ref. 1. The density of platelets is such that a channeled electron encounters ∿25 platelets in traversing the 12-μm-thick Type-Ia diamond. In the (111) direction, the dechanneling probability of an electron in crossing a stacking fault is $\lesssim$1% because of the alternating wide and narrow spacings of the planes (see Ref. 1), whereas in the (110) direction, it is $\gtrsim$15% because there is no such alternation. After ∿25 such crossings, the (111) intensity would be reduced by ∿20% while the (110) intensity would be reduced to virtually nothing.

For the (100) plane, we show the 54.5-MeV data from Ref. 1 in Fig. 3, as well as the present 30.5-MeV data in Fig. 2(c). Here we see a reduction in intensity by a factor of ∿2.5, corresponding to a dechanneling probability of ∿3.5% per platelet encounter. More important, we observe a downshift in energy of the 1 → 0 spectral peak of about 4% for 30.5-MeV electrons and about 8% for 54.5-MeV electrons. For the 54.5-MeV case, the downshift of the 2 → 1 peak is about 3%; this transition is not observable at 30.5 MeV because the n = 2 state is not bound for this case.

## III. THEORETICAL MODEL

The inclusion of atomic thermal vibrations in the derivation of crystalline potentials results in an energy downshift for the deeply-bound states. We have observed this same effect, i.e., an energy downshift, when platelets are introduced into the crystal, which suggests that platelets are similar to thermal vibrations in that they cause an uncertainty in the position of the atoms. Therefore, in our model, to explain the data we assume an effective vibrational amplitude that is the quadrature sum of the actual amplitude and a displacement resulting from the presence of the platelets.

In calculating the theoretical transition energies, we employ the Hartree-Fock potential, modified by a Debye-Waller factor to account for thermal vibrations (see Ref. 3 for the details of how this is done). For the Type-IIa diamond (without platelets), we use the tabulated[14] thermal-vibration amplitude of 0.04 Å. The (100) planar potential so derived is shown as the solid curve in Fig. 4, from which one obtains the calculated transition energies listed in column 3 of Table II. These values agree very well with the measured (100) transition energies for the Type-IIa diamond, listed in column 4 of the table.

The measured (100) transition energies for the Type-Ia diamond, listed in column 5 of Table II, are lower (by 3 to 9%) than the calculated values which use the above value for the thermal-vibration amplitude. When we allow this amplitude to vary, a best fit to the data is achieved for a value of 0.055 Å. This new value produces the calculated (100) transition energies listed in the last column of Table II, and corresponds to the (100) potential shown as the dashed curve in Fig. 4. This result implies that the platelets contribute an equivalent vibrational amplitude of 0.038 Å.

In the preceding derivation, we assumed that the platelets introduced a probability density function for the position of the atoms given by a Gaussian distribution with a standard deviation equal to 0.038 Å. We attempted to use other probability density functions (a uniform distribution and a discrete distribution) as well, but we were unable to match the data. This suggests that the Gaussian function is appropriate.

How reasonable is the 0.038 Å displacement that was calculated? We estimate an average platelet diameter of about 140 Å and a distance of about 4500 Å between platelet encounters along a major plane. This gives a mean displacement of the (100) planes of 0.037 Å for the Lang model and 0.044 Å for the Humble model. These rough calculations indicate that the calculated displacement of 0.038 Å is not unreasonable, and thus that the analysis of channeling-radiation data may lead to a better understanding of the structure of these kinds of aggregate impurities or defects in crystals.

Finally, a comparison can be made between the coherence lengths in the crystal, as obtained from the observed linewidths of the spectral peaks, and the mean distance between platelets determined from infrared-absorption measurements. Assuming a Lorentzian lineshape, the full-width half-maximum (FWHM) linewidth $\Delta E$ is related to the coherence length $\ell_{coh}$ by the relationship $\ell_{coh} = 2\gamma^2\hbar c/\Delta E$.

This comparison is applicable only for the $1 \rightarrow 0$ transition for (100) planes, since this is the only transition for which the spectral peak is not overlapped by other transitions and stands sufficiently above the background to provide an accurate measure of the linewidth. The coherence length is found to be 0.13 μm at a beam energy of 30.5 MeV and 0.17 μm at a beam energy of 54.5 MeV.

The infrared-absorption data indicate a mean separation between platelets of 0.45 μm. If this is taken to be the coherence length for both the n = 0 and n = 1 states, then the coherence length for the 1 → 0 transition is calculated to be 0.22 μm. However, there are other line-broadening mechanisms which tend to reduce $\ell_{coh}$. The most important of these results arises from the thermal vibrations of the atoms; including this effect, the coherence length becomes 0.18 μm. This calculated value is in reasonable agreement with the values obtained from the measured spectral linewidths.

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## REFERENCES


1. H. Park, R. H. Pantell, R. L. Swent, J. O Kephart, B. L. Berman, S. Datz, and R. W. Fearick, J. Appl. Phys. 55, 358 (1984).
2. A preliminary version of these data has been presented in S. Datz, R. W. Fearick, H. Park, R. H. Pantell, R. L. Swent, J. O. Kephart, and B. L. Berman, Nucl. Instrum. Methods B2, 74 (1984).
3. R. K. Klein, J. O. Kephart, R. H. Pantell, H. Park, B. L. Berman, R. L. Swent, S. Datz, and R. W. Fearick, Phys. Rev. B (in press); see also S. Datz, R. W. Fearick, H. Park, R. H. Pantell, R. L. Swent, J. O Kephart, R. K. Klein, and B. L. Berman, Phys. Lett. 96A, 314 (1983).
4. M. Gouanère, D. Sillou, M. Spighel, N. Cue, M. J. Gaillard, R. G. Kirsch, J.-C. Poizat, J. Remillieux, B. L. Berman, P. Catillon, L. Roussel, and G. M. Temmer, Nucl. Instrum. Methods 194, 225 (1982).
5. T. Evans, Contemp. Phys. 17, 45 (1976).
6. A. R. Lang, Proc. Phys. Soc. 84, 871 (1964).
7. P. Humble, Proc. R. Soc. London A381, 65 (1982).
8. J. C. Barry, L. A. Bursill, and J. L. Hutchison, Phil. Mag. (in press). We thank Prof. J. Spence for bringing this latest work to our attention.
9. S. J. Pennycook, Bull. Am. Phys. Soc. 28, 1318 (1983).
10. L. A. Bursill, J. L. Hutchison, A. R. Lang, and N. Sumida, Nature 292, 518 (1981).
11. J. C. Barry, L. A. Bursill, and J. L. Hutchison, Phil. Mag. A48, 109 (1983).

12. G. Davies, Chem. Phys. Carbon 13, 1 (1977).

13. R. W. Fearick and J.P.F. Sellschop, Nucl. Instrum. Methods 168, 195 (1980).

14. D. S. Gemmell, Rev. Mod. Phys. 46, 129 (1974).

Table I. Measured characteristics of 30.5-MeV electron channeling radiation from diamond crystals.

| Plane | Transition | Type IIa (without platelets) | | | Type Ia (with platelets) | | |
|---|---|---|---|---|---|---|---|
| | | Peak energy (keV) | Relative intensity | Width (keV) | Peak energy (keV) | Relative intensity | Width (keV) |
| (111) | Several | 25.0 ± 0.5 | 1.88 | 11.8 ± 0.8 | 24.2 ± 0.6 | 1.27 | 13.3 ± 1.3 |
| (110) | 1 → 0 | 60.1 ± 0.3 | 1.07 | 6.0 ± 0.3 | | | |
| | 2 → 1 | 35.3 ± 0.3 | 0.62 | 5.2 ± 0.3 | No discernible line radiation | | |
| | 3 → 2 | 24.5 ± 0.2 | 0.28 | 4.8 ± 0.3 | | | |
| (100) | 1 → 0 | 43.0 ± 0.3 | 1.00 | 5.9 ± 0.3 | 41.3 ± 0.4 | 0.38 | 10.8 ± 1 |

Table II. Transition energies (in keV) for (100) planes in diamond.

| Electron energy (MeV) | Transition | Calculated with standard potential | Measured | | Calculated with modified potential |
|---|---|---|---|---|---|
| | | | Type IIa | Type Ia | |
| 30.5 | 1 → 0 | 43 | 43.0 ± 0.3[a] | 41.3 ± 0.4 | 41 |
| 54.5 | 1 → 0 | 122 | 119.8 ± 0.7[a] | 111.0 ± 2 | 113 |
| | 2 → 1 | 65 | 64.7 ± 1.5[a] | ∿63 | 63 |

[a]These values supersede the (slightly different) values given in Ref. 1.

## FIGURE CAPTIONS

1. Schematic representations of a platelet in a Type-Ia diamond crystal: (a) according to the model of Lang (Ref. 6), the platelet consists of a double layer of nitrogen atoms; (b) according to the model of Humble (Ref. 7), it consists of a single layer of carbon (or possibly nitrogen) atoms.
2. Channeling-radiation spectra from both Type-Ia (open data points) and Type-IIa (closed data points) diamonds, for 30.5-MeV electrons incident along (a) the (111) planar direction; (b) the (110) planar direction; (c) the (100) planar direction.
3. Channeling-radiation spectra from Type-Ia (open data points) and Type-IIa (closed data points) diamonds, for 54.5-MeV electrons incident along the (100) planar direction.
4. Potentials for the (100) plane in diamond. The solid curve represents the potential which uses the accepted value of 0.040 Å for the thermal-vibration amplitude, as is appropriate for Type-IIa diamonds. The dashed curve represents the potential which uses the value of 0.055 Å, which arises from a best fit to the data for the Type-Ia diamond of the present experiment.

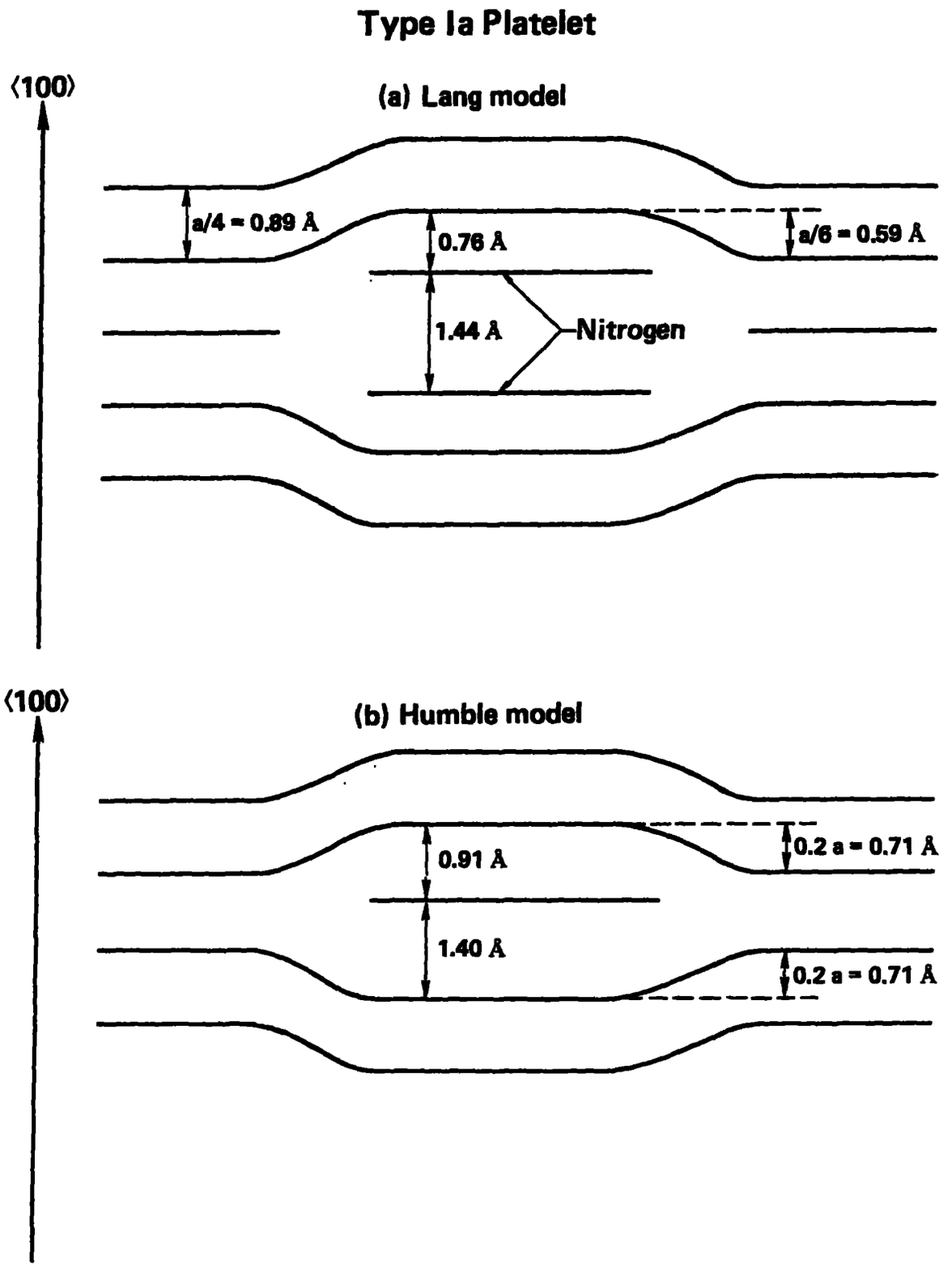
Type Ia Platelet
⟨100⟩
(a) Lang model
a/4 = 0.89 Å
0.76 Å
a/6 = 0.59 Å
1.44 Å
Nitrogen
⟨100⟩
(b) Humble model
0.91 Å
0.2 a = 0.71 Å
1.40 Å
0.2 a = 0.71 Å

Figure 1

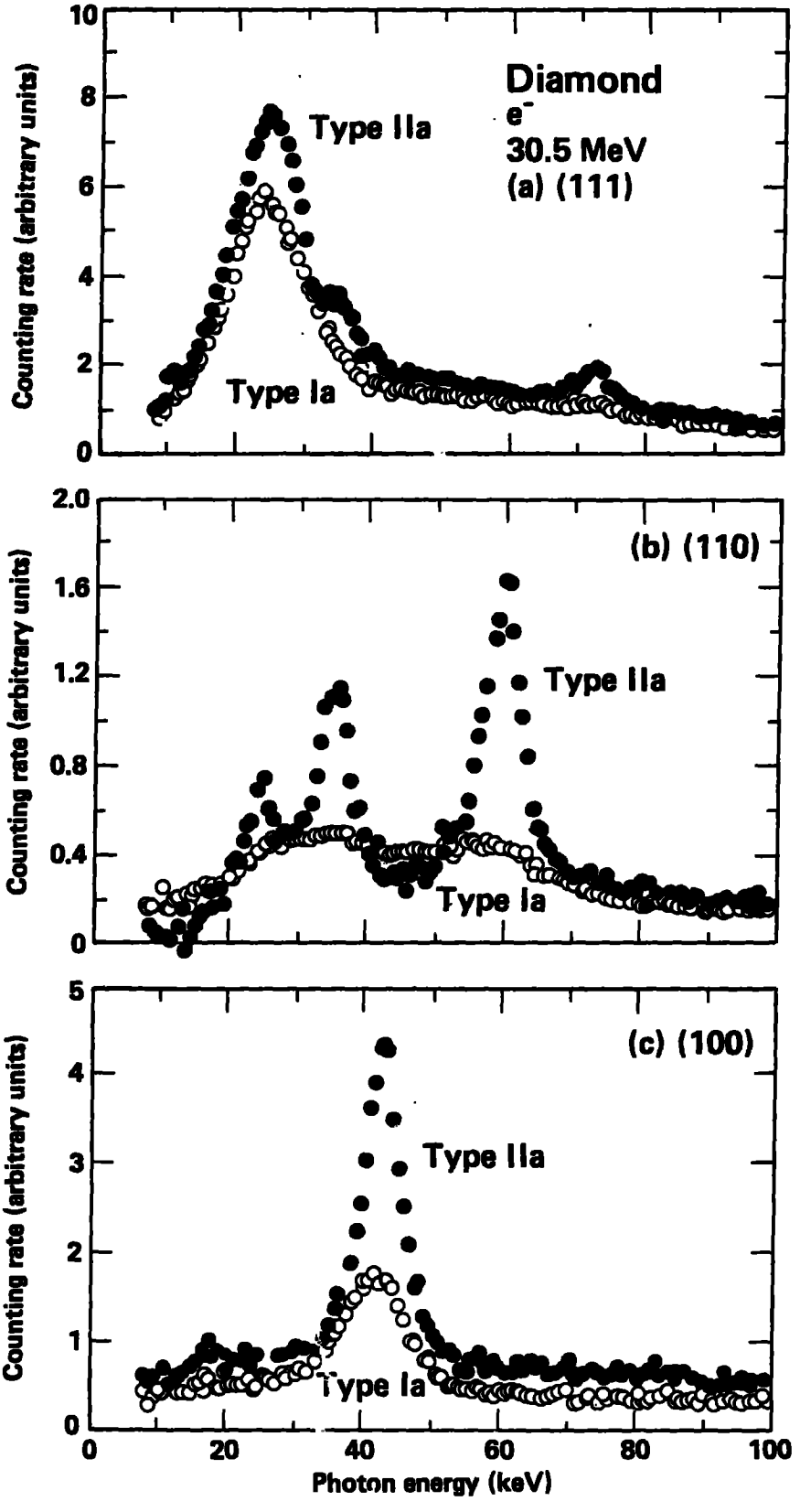
Diamond
e⁻
30.5 MeV
(a) (111)
Type IIa
Type Ia
(b) (110)
Type IIa
Type Ia
(c) (100)
Type IIa
Type Ia
Counting rate (arbitrary units)
Photon energy (keV)
0
20
40
60
80
100

Figure 2

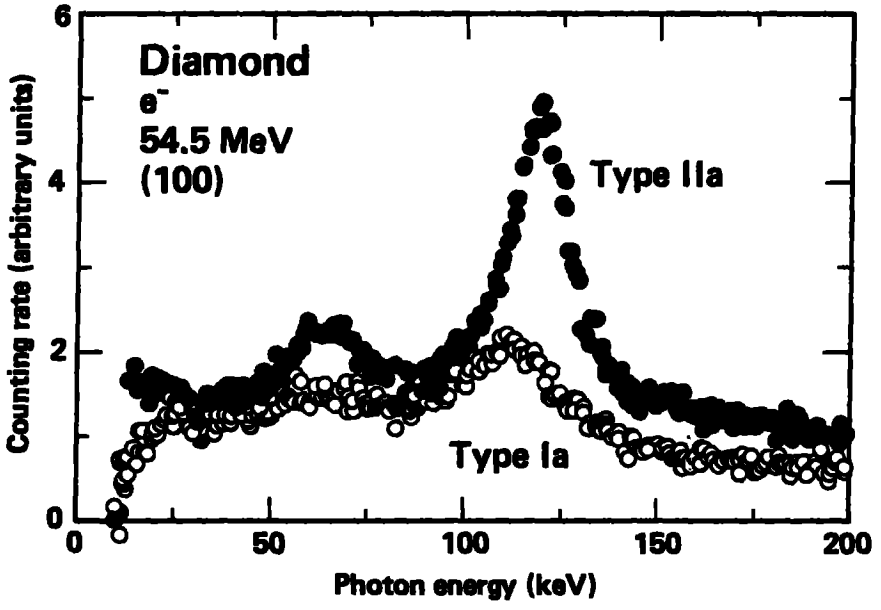
Diamond
e⁻
54.5 MeV
(100)
Type IIa
Type Ia
Counting rate (arbitrary units)
Photon energy (keV)
0
2
4
6
0
50
100
150
200

Figure 3

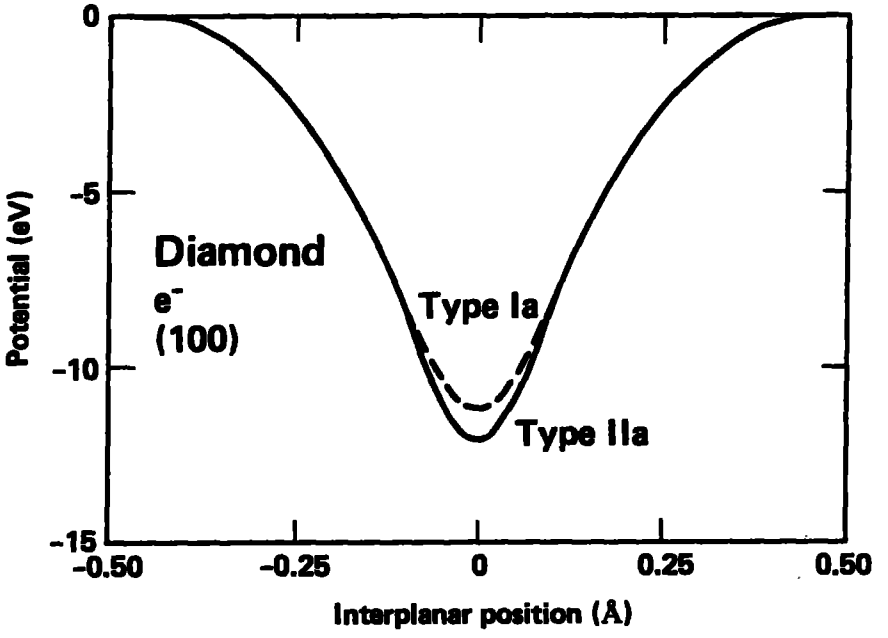
0
-5
-10
-15
Potential (eV)
Diamond
e⁻
(100)
Type Ia
Type IIa
-0.50
-0.25
0
0.25
0.50
Interplanar position (Å)

Figure 4